Characterization of the spray cone angles of fuels with nanoparticle additives

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Abstract

The spray angles produced by fuel nozzles are of interest because they influence the ignition performance and hence the pollutant emissions emanating from fuel spray combustion. Recent studies have indicated that the dispersion of metallic nanoparticles in liquid fuels can affect the fuel spray formation at ambient temperature conditions. Initial results of studies that are evaluating the use of existing phenomenological models to characterize nanofuel sprays are presented here for spray cone angles. Fuel spray cone angles are found to decrease with increasing nanoparticle concentration. These changes are marginal, mainly due to the low nanoparticle concentration values evaluated and ambient conditions of the carrier gas and fuel. These results help to improve the present knowledge of the applicability of such models to nanofuel spray analyses. The suitability of the different models is highlighted and respective implications for their use in nanofuel spray modelling are presented.

Keywords: Spray, atomization, nanofuels, spray cone angle, phenomenological models, nanoparticle additives

Introduction

The need for cleaner sources of energy has become a major global issue owing to global warming and the environmental pollution brought about by conventional fossil fuel usage. To this end and coupled with ever-increasing energy demand, efforts have been made to develop alternative sources of energy as well as improve the existing traditional hydrocarbon fuels. Nanofuels are fuels formed by the dispersion of energetic nanoparticles into conventional fuels. Nanofuels have been found to exhibit improved combustion characteristics compared to conventional fuels. Recent studies have reported increased energy density and low emissions (mainly nitrogen oxide with zero CO_2 and SO_2 emissions) [1 - 6]. Other studies on the thermophysical fuel properties as well as specific combustion sub-processes such as ignition delay and evaporation for multiple base fuel and nanoparticle combinations [7 - 12] have also been carried in an attempt to explain the combustion characteristics of nanofuels. However, the knowledge and understanding of how nanoparticle dispersions in fuels affect the spray and combustion performance in internal combustion engines is still an evolving field.

A good spray dispersion is desirable especially at the pilot injection stage to ensure rapid air-fuel mixing. Too large a spray angle is not desirable as it could lead to losses through fuel impingement on the cylinder walls. The key factors that influence the spray dispersion angle are the nozzle dimensions, injector pressure differential, the liquid fuel properties (density and viscosity) as well as the density of the environment into which the fuel is sprayed. Considering the importance of liquid fuel spray atomization in the overall combustion performance, it is interesting to note that very little work has been done in this area with regards to nanofuels. The studies of Kannaiyan and Sadr [13] and Yamine, *et al*. [14] are among the few available. In the studies, the effects of nanoparticle addition (alumina) with the addition of sorbitan oleate (as a surfactant) on the spray characteristics (spray cone angle, the sheet breakup as well as the ligament characteristics) of Gas-to-liquid (GTL) fuel were investigated. Spray visualization using the shadowgraph technique showed a small decrease in spray angle, and sheet breakup length with increase in nanoparticle concentration. Additionally, enhanced disruption of the sheet ligament coupled with decreased ligament velocity were observed as the nanoparticle concentration was increased. Thus, the reduced spray angle reduces the probability of spray impingement on cylinder walls. Further, the decreased sheet break-up length and ligament velocity, and enhanced ligament disruption ensures quicker droplet formation and a potentially improved combustion performance. The studies were for non-reacting nanofuel sprays and the authors did not present any correlations derived from their experimental data.

Experimental studies can be limited by factors such as cost, safety, time as well as difficult operating conditions. Mathematical models on the other hand have can be used for analyzing complex system processes and sub-processes under variable conditions as well as in the prediction and optimization of system parameters and operations. Mathematical models for engine combustion processes can categorized into three, namely: The Thermodynamic (zero-dimensional), Phenomenological (quasi-dimensional) and the Multi-dimensional models [15]. The phenomenological models are characterized by their ability to provide spatial resolution of the chamber and analyzing and predicting important combustion sub-processes in a timely and less computationally-demanding manner; these have made these models attractive for this study. Phenomenological models for the various engine subprocesses have been developed based on various spatial resolution theories such as the free jet theory [16] and the packet model [17] to analyze and predict characteristics such as the spray tip penetration, for example, and several more exist in literature for the prediction of the spray cone angle, Sauter Mean Diameter (SMD) or droplet size, liquid length, liquid breakup length and time, evaporation rate, ignition delay, reaction time as well as NOx and soot formation [18-31]. None of these have been applied to cases of nanofuel sprays.

With regards to nanofuels, very few mathematical models have been reported in the literature. Gan and Qiao [32] developed a particle aggregation model based on the Population Balanced Equation as a means of explaining the D^2 Law deviation behaviour of nanofuels during evaporation. Statistically based models of the regression analysis equations were reported by Sarvestani *et al*. [33] for predicting the brake specific fuel consumption as well as the emission characteristics of compression ignition engines with respect to nanoparticle concentration (Fe_3O_4) and engine load. Khond and Kriplani [34] also developed a regression model to predict the relationship between evaporation time, rate and temperature as well as the effect of particle loading using carbon nanotube blended emulsified neem biodiesel. A Genetic Programming (GP) based model approach was also reported by Ghanbari *et al*. [4] in predicting the combustion performance and emission parameters.

The focus of the work presented in this paper is the elucidation of the applicability of existing internal combustion phenomenological models to nanofuel spray analysis, in this case, the spray cone angle. This has hitherto not been studied.

Methodology

Experimental Data

The fuel data for this study were extracted from the experimental investigations of Kannaiyan and Sadr [13] and Yamine, *et al*. [14]. The details are provided in Table 1 below.

Table 1. Fuel Data [13, 14]

Properties	**Base fuel** (Gas-to-liquid (GTL) fuel)	**Nanofuels (**Base fuel + alumina nanoparticles**)**			
		Nanoparticle compositions			
		0.5%	1.0%	1.5%	2.0%
Density (kg/m^3)	750.9	754.9	757	762.9	763.6
Dynamic Viscosity (cP)	1.005	1.011	1.016	1.02	1.02
Surface Tension (N/m)	0.024	0.02362	0.02328	0.02315	0.02315

In the experiments [13, 14], a pressure swirl nozzle with an orifice diameter, D = 0.8mm, was used. Injection pressure values of 0.3 (used for this study) and 0.9 MPa, typical of an aircraft engine operating cycle were maintained, with the ambient gas density, ρ_g , at 3.39kg/m^3. The base fuel was pure gas-to-liquid fuel and the nanofuel was the base fuel with the dispersion of Al_2O_3 (alumina) nanoparticles at weight concentrations of 0.5%, 1%, 1.5% and 2%. Sorbitan mono-oleate, 0.4% volume concentration in all three cases, was used as the surfactant to ensure the stability of the nanofuel solutions. The fuels were injected into quiescent ambient atmospheric conditions. The shadowgraphy technique was used to acquire the spray cone angle, liquid sheet breakup length and velocity from images of the spray. The images were processed using image-processing programs.

The Models

Six phenomenological spray cone angle models developed over the last 35 years were selected for this study. A set of the models are for those developed for pressure swirl atomizers, as used in the experiments. A second set of models is based on plain orifice atomizers to ascertain if these models can predict the qualitative trend of nanofuel spray cone angles.

Pressure swirl atomizers

Lefebvre Model (1989)

This model considers the influence of fuel properties as well as injection pressure as given in equation (1). It was modelled after the operation of pressure swirl atomisers [28].

$$2\theta = 6 \times k^{-0.15} \times (\frac{\Delta P \times D^2 \times \rho_l}{\mu_l^2})^{0.11} \tag{1}$$

Where k is the atomiser constant given by;

$$k = \frac{A_p}{D \times d_{sw}} \tag{2}$$

Taking a value of k = 0.02 [36], and substituting the other known values into equation (1), the spray cone angle was obtained as a function of liquid fuel density and viscosity, given as

$$2\theta = 8.998 \times \frac{\rho_l^{0.11}}{\mu_l^{0.22}} \tag{3}$$

Ballester - Dopazo Model (1994)

This correlation presented in equation (4) was modelled based on heavy oil flow through simplex pressure swirl atomizers [39].

$$2\theta = 16.156 \times K^{-0.39} \times D^{1.13} \times \mu_l^{-0.9} \times \Delta P^{0.39} \tag{4}$$

Where k is the atomiser constant given in equation (2).

Taking k = 0.02 [36], and substituting the other known values into equation (4), the spray cone angle was obtained as a function of the liquid fuel density and viscosity as follows,

$$2\theta = 88.6 \times \mu_l^{-0.9} \tag{5}$$

Plain orifice atomizers

Varde – Popa Model (1984)

This correlation which is presented in equation (6) was modelled to represent the operation of high pressure diesel sprays in plain orifice atomizers [35].

$$tan\theta = \gamma(\frac{\rho_g}{\rho_l})^{0.33} \tag{6}$$

Where, γ is a constant of proportionality which also serves as a multiplier and was assumed to be 1.5 in this study in order to obtain results in the range of the plain orifice atomizer cone angle. On substituting these values into the model as shown in equation (6), the spray cone angle, 2θ as a function of the liquid fuel density was obtained as,

$$2\theta = 114.59tan^{-1}(2.244\rho_l^{-0.33}) \tag{7}$$

Hiroyasu Model (1990)

The Hiroyasu spray cone angle model [37] is given as;

$$\theta = 83.5 \times \left[\frac{L}{D}\right]^{-0.22} \times \left[\frac{D}{D_0}\right]^{0.15} \times \left[\frac{\rho_g}{\rho_l}\right]^{0.26} \tag{8}$$

It is evident that most of the parameters needed for this model are concerned with nozzle dimensions and since some of these data were not available in the referred experimental work, justifiable assumptions were thus made as follows. Since this model represents a plain orifice atomizer, a typical nozzle aspect ratio, L/D = 4.2 was adopted. Using the sac dimensions from the experimental work of Siebers [38], the sac chamber diameter, D_0 = 0.916mm was obtained.

Substituting these values into the model, spray cone angle, 2θ as a function of the liquid fuel density was obtained as,

$$2\theta = 161.76 \times \rho_l^{-0.26} \tag{9}$$

Delacourt Model (2005)

This correlation [40] given in equation (10) was modelled for plain orifice nozzles.

$$2\theta = \frac{360}{\pi} tan^{-1}(B(\frac{\rho_g}{\rho_l})^m) \tag{10}$$

Where, $B = 0.31, m = 0.2$

On substituting these values into equation (10),

$$2\theta = 114.59tan^{-1}(0.396\rho_l^{-0.2}) \tag{11}$$

Zeng Model (2012)

This model is a product of dimensional analysis of multi-hole spray characteristics [41] and is given as

$$\theta = 0.273(\frac{\rho_g}{\rho_l})^{0.287} \times We^{0.46} \tag{12}$$

On substituting known and given parameters into equation (12), equation (13) was obtained as a function of the fuel properties;

$$2\theta = 13.282 \times \rho_l^{-0.287} \times \sigma^{-0.46} \tag{13}$$

Results and Discussion

Pressure Swirl Atomizer Model Results

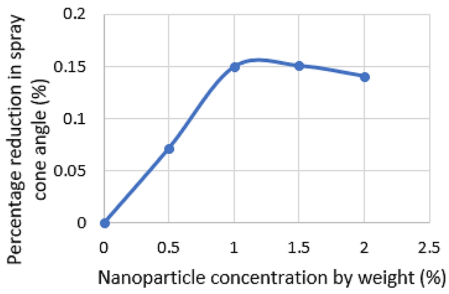

Figure 1. Lefebvre Model.

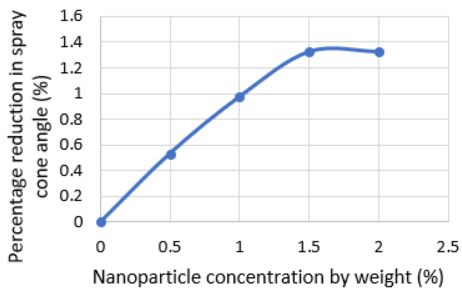

Figure 2. Ballester and Dopazo Model

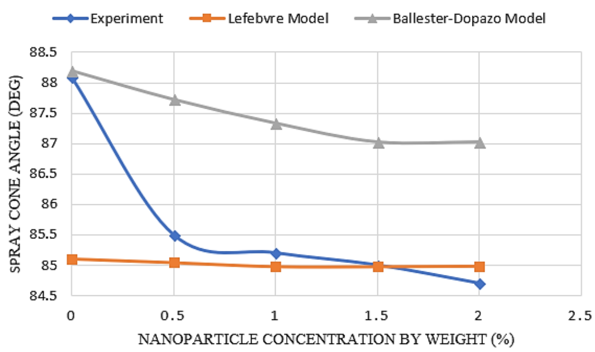

Figure 3. Comparison of Pressure swirl models; spray cone angles.

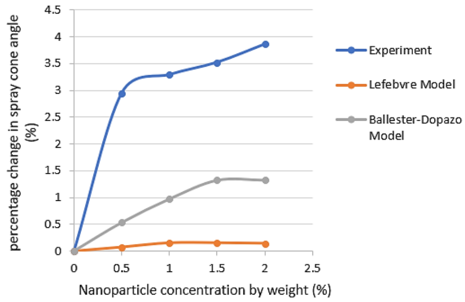

Figure 4. Comparison of Pressure swirl models; percentage change in spray cone angles.

Results presented in Figures 1- 4 show decreasing spray cone angle values with increasing nanoparticle concentration by weight values for both the experimental data and the pressure swirl atomizer models. This is mainly due to the increase in the fuel density values brought about by the addition of the nanoparticles (Table 1). In all cases, the decrease in the spray cone angle values is halted between the 1.5% and 2% nanoparticle concentration by weight cases as increasing the nanoparticle concentration beyond 1.5% by weight increases the fuel density by less than 0.01%.

In the Lefebvre [28] and Ballester- Dopazo [39] correlations, represented in equations (1) and (4) respectively, the spray cone angle dependence includes the nozzle characteristics, the liquid fuel density and viscosity as well as the injection pressure. With respect to the fuel parameter effect, it can be clearly seen in the model equations that the viscosity has an effect on the spray cone. This fact clearly explains the marginal cone angle increase observed in Figures 1 and 2 for the 2% nanoparticle concentration cases. This increase is due to the zero change in the viscosity on increasing the nanoparticle concentration as shown in the experimental data (Table 1). Lefebvre [28] explained that this was as a result of the reduction in the flow tangential velocity brought about by the frictional force due to the velocity differences between the liquid layers (within the liquid as well as with respect to the nozzle walls).

A comparison of all the two models with the experimental results of Kannaiyan and Sadr [13] and Yamine, *et al*. [14] as presented in Figures 4 and 5 show a clear agreement in terms of the general decreasing effect of the spray cone angle with increasing nanoparticle concentration though the details differ. It is important to note that the rate of change of spray cone angle predicted by the six spray cone angle models as well as the actual experimental data is marginal as observed in figures 3 and 4; the nanoparticle concentration in the nanofuel solution was low and the dispersal conditions were ambient. However, from figures 3 and 4, the initial drop in spray cone angle (at 0.5% wt nanoparticle concentration) is more marked in the experiments compared to the model predictions. Spray cone angle values predictions for the swirl atomizer models were are at least 97% of the corresponding values obtained from the experimental work. Therefore, the spray cone angle phenomenological models developed for diesel fuel spray cases can be applied for nanofuels spray cases.

Plain Orifice Atomizer Model Results

Can the plain orifice atomizer model capture the same qualitative trends for the spray cone angle as the experimental data?

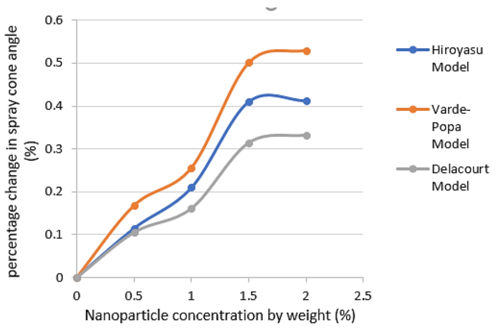

Figure 5. Comparison of Plain orifice models; percentage change in spray cone angles.

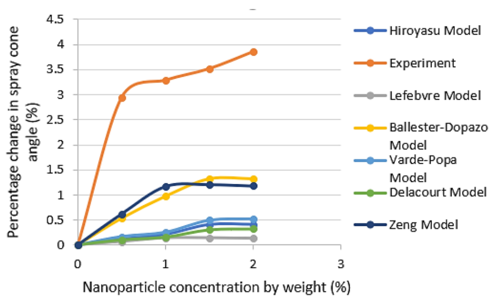

Figure 6. Comparison of all the models; percentage change in spray cone angles.

From figures 5 and 6, for five cases the decrease in the spray cone angle values is halted between the 1.5% and 2% nanoparticle concentration by weight cases. Conversely, an increase in the spray cone angle was obtained for the case of the Zeng [41] model (Figure 6) for increasing nanoparticle concentration values. The correlation for the Zeng [41] model (equation (12)) includes the Weber number, hence, surface tension reduction with increasing nanoparticle loading rate (see Table 1) leads to increased Weber number values thus increasing the spray cone angle. The plain orifice models, Varde – Popa [35], Hiroyasu [37], Delacourt [40] and Zeng [41] suggest, to varying degrees, a spray cone angle dependence on the ambient gas and liquid fuel density values. They do not consider other key factors affecting the cone angle as explained by Lefebvre [28] such as the fuel viscosity and the injection pressure. Also the rate of change of spray cone angle predicted by all the models is also marginal as observed in Figure 5. Overall, from figure 6, both the plain orifice and pressure swirl models predict marginal decreases in the value of the spray cone angle with increases in the nanoparticle concentration in nanofuels.

Summary and Conclusions

The applicability of diesel fuel spray phenomenological models to nanofuels fuel sprays for the prediction of spray cone angle values was evaluated. Six different models developed in the past 35 years as well as experimental nanofuel spray cone angle data were used for the study. The predicted results from the models indicate that the spray cone angle decreases with increasing nanoparticle concentration thus, similar to the trend obtained from the experimental results. Thus in cases where wetting of the cylinder walls is undesirable, this could be a useful way of achieving this. For the experimental conditions presented in this study (quiescent, ambient, atmospheric), the the spray cone angle phenomenological models developed for diesel fuel spray cases for pressure swirl atomizers can be applied for nanofuels spray cases. The implications include that these types of atomizers do not need to be modified when nanofuels are used at these operating conditions. The models for the plain orifice atomizers can predict the spray cone angle trend with respect to nanoparticle concentration in the nanofuel solution. Thus the prediction of the other nanofuel spray characteristics under these conditions using existing phenomenological models will explored. However, under spray combusting conditions, it is likely that new models would be need to be developed, as the nanoparticles present in the fuels react differently at these conditions.

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Nomenclature

A - Area (mm^2)
ΔP - Nozzle pressure drop (MPa)
D - Orifice diameter (mm)
L/D - Nozzle aspect ratio
D_o - Needle diameter/ sac chamber diameter (mm)
d - Diameter (mm)

Greek Nomenclature
ρ - Density (g/L)
θ - Half angle of the spray cone (degrees)
2θ - Spray cone angle (degrees)
γ, k - Constant terms
μ - Viscosity (Pa-s)
σ - Surface tension (N/m)

Subscripts
l - Liquid phase
g - Gas
p - Swirl port
sw - Swirl chamber

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